Ergodicity and mixing in quantum dynamics

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After a brief historical review of ergodicity and mixing in dynamics, particularly in quantum dynamics, we introduce definitions of quantum ergodicity and mixing using the structure of the system's energy levels and spacings. Our definitions are consistent with the usual understanding of ergodicity and mixing. Two parameters concerning the degeneracy in energy levels and spacings are introduced. They are computed for right triangular billiards and the results indicate a very close relation between quantum ergodicity (mixing) and quantum chaos. At the end, we argue that, besides ergodicity and mixing, there may exist a third class of quantum dynamics which is characterized by a maximized entropy.

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I. INTRODUCTION

Ergodicity and mixing are of fundamental importance in statistical mechanics. Ergodicity justifies the use of a microcanonical ensemble and mixing ensures that a system approaches equilibrium dynamically [1]. However, it is difficult to prove with mathematical rigor that a classical dynamical system is ergodic or mixing. As a result, the microcanonical ensemble in textbooks is still established with postulates [2]. More importantly, the concept of ergodicity and mixing is now obsolete in the following sense: they are defined for classical dynamics, while the dynamics of microscopic particles are fundamentally quantum. To establish statistical mechanics with quantum dynamics, we need to define ergodicity and mixing in quantum dynamics.

In this work we define quantum ergodicity and mixing using the structure of the system's energy levels and spacings without any assumption. With the early results of von Neumann [3,4] and Reimann [5], it can be shown that our definitions, which appear very mathematical, do lead to the usual understanding of ergodicity and mixing. We introduce two parameters to characterize the degeneracy in energy levels and spacings, respectively. They are computed numerically for right triangular billiards, whose classical dynamical properties have been studied in great detail [6,7]. The numerical results indicate that there is a very close relation between quantum chaos and quantum ergodic or mixing: most nonintegrable finite quantum systems are both ergodic and mixing. It is clear from this example that a system whose quantum dynamics is ergodic may not be ergodic in the corresponding classical dynamics.

We draw a parallel between our paper and Peres's two papers [8,9]. Peres introduced his definitions for quantum ergodicity and mixing in the first paper [8], then, with his coauthors, illustrated these two concepts with examples in the second paper [9]. In our paper we do both: we first introduce our definitions for quantum ergodicity and mixing and then illustrate them with examples.

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II. QUANTUM ERGODICITY AND MIXING

A. History

Ergodicity was introduced by Boltzmann in 1871 as a hypothesis to understand thermodynamics microscopically [1]. Mixing was first discussed by Gibbs [10] and its mathematical definition was introduced by von Neumann in 1932 [11]. Both concepts concern the long-time behavior of dynamical systems and are of fundamental importance to statistical mechanics. They are now the focus of a fully developed branch of mathematics called ergodic theory [12,13]. However, ergodicity and mixing are becoming less interesting to physicists for two reasons: (i) After decades of research with many meaningful results [12,13], it is still not rigorously proved that many of the physical systems existing in nature are either ergodic or mixing. (ii) Both ergodicity and mixing are only defined for classical systems, while microscopic particles are fundamentally quantum. Therefore, it is imperative to define both ergodicity and mixing in quantum systems.

The first physicist who discussed quantum ergodicity was von Neumann. In 1929, von Neumann proved two inequalities, which he named the quantum ergodic theorem and quantum H theorem [4], respectively. His ergodic theorem ensures that the long-time average of a macroscopic observable not only equals its microcanonical ensemble average but also has small fluctuations. In other words, the observable deviates considerably from its averaged value only rarely. So, by ergodicity, von Neumann actually meant both ergodicity and mixing. Interestingly, mixing as defined for classical dynamics was only introduced three years later, in 1932, by von Neumann [11]. In addition, according to von Neumann's H theorem, once the quantum system dynamically relaxes to its equilibrium state, where macroscopic observables have small fluctuations, this state also has a maximized entropy.

von Neumann's results have been criticized by many [8,14]. We share the view of Goldstein *et al.* [14] that the criticism was mostly misguided; von Neumann had captured the essence of quantum ergodicity and mixing and his results are inspirational. Nevertheless, some issues with von Neumann's results do exist. Most of the variables involved in the two theorems are not computable in principle [15]. The reason is as follows.

To prove his theorems, von Neumann introduced a coarse-graining, which groups the Planck cells in quantum phase space into some big cells. All the microscopic states in one group of Planck cells correspond to a single macroscopic state. This kind of coarse-graining is certainly reasonable. However, no one knows how to technically establish such a many-to-one mapping between macroscopic state and microscopic state. This makes many of von Neumann's variables in Ref. [4] uncomputable. Though there may have been some revisions to the theorem [16], this difficulty has not been overcome.

More recent definitions of ergodicity and mixing in quantum mechanics were given by Peres [8]. Peres recalled the behavior of dynamical variables in classical ergodic and mixing systems and expected that there should be analogous behavior in quantum ergodic and mixing systems. In accordance with von Neumann's results, Peres defined ergodicity as the time average of any quantum operator equal to its microcanonical ensemble average and mixing as any quantum operator having small fluctuations. However, Peres's definitions were based on his own definition of quantum chaos [8], which is a subject of debate itself. To define quantum chaos, Peres used an ambiguous concept of pseudorandom matrix. These two steps, which are not mathematically very rigorous, along with other reasonable but ambiguous assumptions, render Peres's definitions not satisfactory.

In the literature quantum ergodicity has been studied from a different perspective, where the concept "quantum ergodicity" is regarded as a branch of quantum chaos [17–26]. This group of researchers mainly focused on how the eigenfunctions of a Hamiltonian converge to equidistribution in classical phase space in the semiclassical limit or high-energy limit, with little discussion of the dynamical behavior of a quantum system. Their definitions of quantum ergodicity and mixing rely on the corresponding classical cases and thus are not genuinely quantum mechanical. Srednicki's work on eigenfunction thermalization follows along this line and has little discussion of quantum dynamics [27].

In the following subsection we define quantum ergodicity and mixing using the energy structure of the system, that is, eigenenergies and their spacings. Our definitions are mathematically precise and have no assumptions. Furthermore, by following von Neumann [3] and Reimann [5], we can show that our definitions lead to the usual physical understanding of ergodicity and mixing. Our definitions are based on quantum dynamics and expressed in the language of pure quantum mechanics without referring to classical mechanics. Near the end of this paper, based on a recent work [15], we argue that we may be able to expand our definitions to include a third class of quantum dynamics, which is characterized by a maximized entropy.

B. Definitions

Consider a quantum system with discrete eigenenergies $\{E_n\}$ and corresponding energy eigenstates $\{|\phi_n\rangle\}$.

Ergodicity. A quantum system is ergodic if its eigenenergies satisfy

$$\delta_{E_m,E_n} = \delta_{m,n}. \tag{1}$$

Mixing. A quantum system is mixing if its eigenenergies satisfy both the above condition, Eq. (1), and the following condition:

$$\delta_{E_k-E_l,E_m-E_n} = \delta_{k,m}\delta_{l,n}, \quad \text{for} \quad k \neq l, \quad m \neq n\,. \tag{2}$$

Condition (1) indicates that there is no degenerate eigenstate. Condition (2) implies that there is no degeneracy in energy gaps between any pair of eigenenergies. It is clear that a quantum system that is mixing must be ergodic, similar to classical dynamics. As we show in the following, condition (1) can lead to the usual intuitive understanding of ergodicity: the long-time average equals the ensemble average. With both conditions, Eq. (1) and Eq. (2), one can show that the so-defined mixing indeed means a small time fluctuation for an observable.

Suppose that the quantum system is in the initial state $|\psi(0)\rangle = \sum_n c_n|\phi_n\rangle$. After evolving for a period of time t, the quantum system is in a state described by $|\psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|\phi_n\rangle$. For an observable $\hat{A}$, its expectation value at time t is given by

$$\langle\hat{A}(t)\rangle \equiv \langle\psi(t)|\hat{A}|\psi(t)\rangle = \mathrm{tr}\hat{A}\hat{\rho}(t), \tag{3}$$

where $\hat{\rho}(t) \equiv |\psi(t)\rangle\langle\psi(t)|$ is the density matrix at time t. Its long-time average is

$$\langle\hat{A}\rangle_T \equiv \lim_{T\to\infty}\frac{1}{T}\int_0^T\langle\hat{A}(\tau)\rangle d\tau. \tag{4}$$

We now introduce a density matrix:

$$\hat{\rho}_{\mathrm{mc}} \equiv \sum_n |c_n|^2|\phi_n\rangle\langle\phi_n|. \tag{5}$$

This density matrix does not change with time and it can be regarded as describing a microcanonical ensemble [3,5,15]. This allows us to define the ensemble average as

$$\langle\hat{A}\rangle_E \equiv \mathrm{tr}\hat{A}\hat{\rho}_{\mathrm{mc}}. \tag{6}$$

For a quantum system satisfying condition (1), it is easy to check that [3,8] (see also Appendix B)

$$\langle\hat{A}\rangle_E = \langle\hat{A}\rangle_T; \tag{7}$$

that is, the long-time average of $\hat{A}$ equals its microcanonical ensemble average.

For a quantum system satisfying both conditions, Eq. (1) and Eq. (2), one can prove [5,28] that the long-time averaged fluctuation F_A^2 satisfies (see also Appendix B)

$$F_A^2 \equiv \frac{\langle|\langle\hat{A}(t)\rangle - \langle\hat{A}\rangle_E|^2\rangle_T}{\|\hat{A}\|^2} \leqslant \mathrm{tr}\hat{\rho}_{\mathrm{mc}}^2, \tag{8}$$

where $\|\hat{A}\|^2 = \sup\{\langle\psi|\hat{A}^\dagger\hat{A}|\psi\rangle : |\psi\rangle \in \mathscr{H}\}$ is the upper limit of the expectation value of $\hat{A}^2$ in the Hilbert space. This demonstrates that a mixing quantum system indeed has small time fluctuations.

A few remarks are warranted here to put our definitions in perspective.

Remark 1. Our definitions of ergodicity and mixing for quantum systems are mathematically very precise. They do not involve any concepts or assumptions, which are mathematically ambiguous. Peres made many assumptions in his definitions [8], which are reasonable but ambiguous mathematically. In particular, we do not need to define quantum chaos first as Peres did [8].

Remark 2. Although our definitions appear very mathematical, as we have shown, they are consistent with the familiar physical pictures that we have had with ergodicity and mixing in classical dynamics: ergodicity means that the long-time average equals the ensemble average; mixing implies small time fluctuations. Moreover, similarly to the classical case, a quantum mixing system is ergodic, but not vice versa.

Remark 3. Our definitions have their roots in the 1929 paper where von Neumann proved a quantum ergodic theorem [3]. However, in 1929 von Neumann did not distinguish ergodicity and mixing. His view of ergodicity at that time is closer to the current view of mixing. In other words, his quantum ergodic theorem might be better called the quantum mixing theorem.

It is worthwhile to note two interesting points: (i) von Neumann used both condition (1) and condition (2) to prove his quantum ergodic theorem; and (ii) mixing in classical dynamics was introduced three years later, in 1932, by von Neumann himself [11].

Remark 4. The density matrix $\hat{\rho}_{\rm mc}$ is used as the microcanonical ensemble in the above discussion. It is not the standard microcanonical ensemble found in textbooks [2],

$$\hat{\rho}_{\rm tb} = \frac{1}{N} \sum_{E_n \in [E, E+\delta E]} |\phi_n\rangle\langle\phi_n|, \tag{9}$$

where N is the number of energy eigenstates in the energy interval $[E, E+\delta E]$. However, we can certainly choose an initial state such that $|c_n|^2 = 1/N$ for $E_n \in [E, E+\delta E]$ and $|c_n| = 0$ otherwise. In this way, we recover the textbook microcanonical ensemble $\hat{\rho}_{\rm tb}$. That is, $\hat{\rho}_{\rm tb}$ is just a special case of $\hat{\rho}_{\rm mc}$.

Remark 5. Our definitions of ergodicity and mixing for quantum systems are independent of the initial conditions. Nevertheless, to thoroughly understand them, we do need to consider initial conditions, as the density matrix $\hat{\rho}_{\rm mc}$ depends on the initial conditions. While Eq. (7) and Eq. (8) hold for an arbitrary initial condition, not all of the initial conditions are of physical interest. If we choose an initial state where only a few eigenstates are occupied, not only is it no longer sensible to regard $\hat{\rho}_{\rm mc}$ as a microcanonical ensemble, but also the fluctuation F_A^2 in Eq. (8) is not small. However, this kind of initial condition is hard to realize in experiments or to find in nature for a many-body quantum system. Physically, when a many-body quantum system is excited by a practical means, it usually enters into a quantum state where a large number of eigenstates are occupied. This is also the reason that the standard microcanonical ensemble $\hat{\rho}_{\rm tb}$, which looks quite artificial, works well as long as the system is large.

This aspect is quite similar to classical systems. In an ergodic or mixing classical system there always exist solutions which are not ergodic or mixing, for example, the periodic orbits. However, these nonergodic or nonmixing solutions are rare or have measure 0 in rigorous mathematical language so that the overall properties of the system are not affected.

Remark 6. Many quantum systems have certain symmetries and, correspondingly, some good quantum numbers. Energy degeneracy can easily occur between the eigenstates of different symmetric sectors. As a result, these quantum systems are in general not ergodic and mixing. However, if one focuses only one symmetric sector, the quantum system can be ergodic or mixing. In this case, we may say that the quantum system is ergodic or mixing in a sub-Hilbert space.

Remark 7. Although classical ergodicity and mixing are of fundamental importance in statistical mechanics, their definitions can be applied to single-particle systems. Similarly, our definitions can be applied to single-particle quantum systems.

To conclude our definitions we offer two simple and illustrative examples. The first is the one-dimensional harmonic oscillator. There is no energy degeneracy so it is ergodic. There is a great deal of degeneracy in energy spacings so that it is not mixing. Interestingly, for the classical dynamics, the one-dimensional harmonic oscillator is similar: it is ergodic but not mixing.

The second example is a particle in a one-dimensional box system, where there is degeneracy neither in energy levels nor in energy spacings. According to our definitions, it is both quantum ergodic and mixing. It is not difficult to find that its classical counterpart is indeed both ergodic and mixing [29].

C. Degeneracy parameters

There has been a tremendous amount of work on quantum chaos or quantum nonintegrability [30]. It is interesting to see how our quantum ergodicity or mixing is related to quantum chaos. In other words, are the two conditions, Eq. (1) and Eq. (2), easy to satisfy in quantum chaotic systems?

On the other hand, it is also interesting to know how infrequent exceptions to these two conditions affect quantum dynamics. When a quantum system has a relatively small number of degeneracies, then almost all of its states contain either no degenerate eigenstates or only a few. For the former, Eq. (7) still holds; for the latter, the left-hand side of Eq. (8) differs from the right-hand side only slightly. So, in a practical sense, this quantum system is ergodic. The situation is similar for mixing: infrequent degeneracy in the energy gap is not important. von Neumann had a similar point of view [3]. Short and Farrelly showed quantitatively how infrequent degeneracy is not important [31].

To address the above two issues, we introduce two parameters, ζ and ξ, which describe the average degeneracy in energy levels and average degeneracy in energy level spacings, respectively, for a given finite set of energy levels. The parameter ζ is defined as

$$\zeta = \frac{1}{N} \sum_{m,n} \left(\delta_{E_m, E_n} - \delta_{m,n}\right), \tag{10}$$

where N is the number of energy levels in the set. The other parameter, ξ, is defined as

$$\xi = \frac{1}{N(N-1)} \sum_{k \neq l, m \neq n} \left(\delta_{E_k - E_l, E_m - E_n} - \delta_{k,m}\delta_{l,n}\right). \tag{11}$$

Furthermore, it is useful to define two distribution functions, $f(\epsilon)$ and $g(\Delta)$. $f(\epsilon)$ is the probability of the eigenenergies having value ϵ; $g(\Delta)$ is the probability of the energy level spacings at Δ. With the aid of these distribution functions, we can reformulate the definitions of ζ and ξ, respectively, as

$$\zeta = N\sum_{\epsilon} f^2(\epsilon) - 1, \tag{12}$$

$$\xi = N(N-1)\sum_{\Delta} g^2(\Delta) - 1. \tag{13}$$

These two functions are clearly related; their explicit relation is

$$\begin{aligned} g(\Delta) &= \sum_{\epsilon} f(\epsilon)\frac{Nf(\epsilon+\Delta)-\delta_{\Delta,0}}{N-1} \\ &= \frac{N}{N-1}\sum_{\epsilon} f(\epsilon)f(\epsilon+\Delta) - \frac{\delta_{\Delta,0}}{N-1}. \end{aligned} \tag{14}$$

We clarify that in our definition Δ can be negative. In other words, for two arbitrary energy levels, E_m and E_n, with $m \neq n$, $E_m - E_n$ and $E_n - E_m$ give rise to two energy level spacings rather than one. We also emphasize that our definitions of ζ and ξ are for a given set of energy levels, not for all the energy levels in the system. The reason is that only a finite set of energy levels is involved in any meaningful physical process.

According to these definitions, the two conditions, Eq. (1) and Eq. (2), are equivalent to $\zeta \equiv 0$ and $\xi \equiv 0$, respectively. The larger ζ (or ξ) is, the more strongly the nondegenerate-energy condition, Eq. (1) [or the nondegenerate-gap condition, Eq. (2)], is violated. We anticipate that for small ζ and ξ quantum systems can still be regarded as ergodic or mixing. For systems where ζ and ξ are strictly equal to 0, we say that they are *ideal* ergodic systems or *ideal* mixing systems.

III. MODEL

In this section we use an example to illustrate our concepts of quantum ergodicity and mixing. We consider the motion of one particle with mass m in a right triangular billiard, as shown in Fig. 1. Mathematically, this billiard is described by the following potential

$$V(x,y) = \begin{cases} 0 & 0 < x < l,\ 0 < y < \alpha x, \\ \infty & \text{otherwise.} \end{cases} \tag{15}$$

Without loss of generality, we restrict ourselves to $\alpha \geqslant 1$ or $0 < \theta \leqslant \pi/4$ ($\alpha = \cot\theta$). It is interesting to note that this billiard system is equivalent to the system of two hard-core particles moving in a one-dimensional square potential with infinite walls [7].

We choose this simple model for two reasons. (i) We can study both the integrable cases and the chaotic cases by adjusting α. (ii) Many meaningful results on classical ergodicity and mixing in this model have been obtained previously [6,7], and we can compare them to our quantum results. Other models such as the Bose-Hubbard model [32] do not have the above advantages.

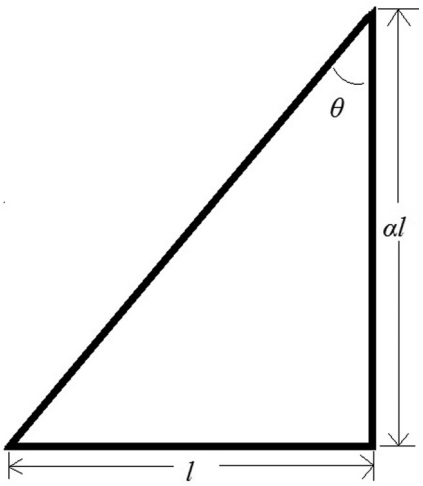

FIG. 1. A right-triangle billiard. Without loss of generality, we take $\alpha \geqslant 1$ or, equivalently, $0 < \theta \leqslant \pi/4$.

The classical integrability of this model is well known. The system is integrable only when $\theta = \pi/4$ or $\theta = \pi/6$ (equivalently, $\alpha = 1$ or $\alpha = \sqrt{3}$). When $\theta = \pi M/N$, where M and N are two coprime integers and $(M,N) \neq (1,4),(1,6)$, the system has two independent invariants. However, it is regarded as pseudointegrable [33–35] because the invariant surface of classical motion in phase space has a genus $2 \leqslant g < \infty$ (it is integrable only when the genus $g = 1$). For all other values of θ, the triangle system has only one invariant and is generally regarded as chaotic.

To study the quantum dynamics of this model, we need to calculate the eigenenergies and eigenstates. This can be done only numerically for an arbitrary value of parameter α. We use the exact diagonalization method (see Appendix A for details). In our calculation, we choose $h = m = l = 1$. In addition, to avoid confusion, we use the single parameter α (instead of θ) to represent the shape of the triangle billiard in the following discussion.

IV. DISTRIBUTIONS OF ENERGY LEVELS

In Sec. II we have defined quantum ergodicity and mixing with two conditions, Eq. (1) and Eq. (2), regarding the distribution of the system's energy levels. In this section, we examine to what extent these two conditions are satisfied by the triangle billiard and how they are related to the integrability of this model via parameters ζ and ξ. In the next section, we show that the quantum dynamics of the triangle billiard are dictated by these two conditions.

The study of quantum chaos has revealed that the structure of quantum energy levels of a system is closely related to the classical integrability of the system [8,36]. One often uses the nearest spacing distribution (NSD) $p(s)$ of a system to describe its structure of quantum energy levels, where $s > 0$ is the spacing between two nearest energy levels. The following feature of the NSD is well known. For a system whose classical dynamics is integrable, its NSD is Poisson-like, with a peak distribution at $s = 0$. For a system whose classical dynamics is chaotic, the NSD of its quantum energy levels is

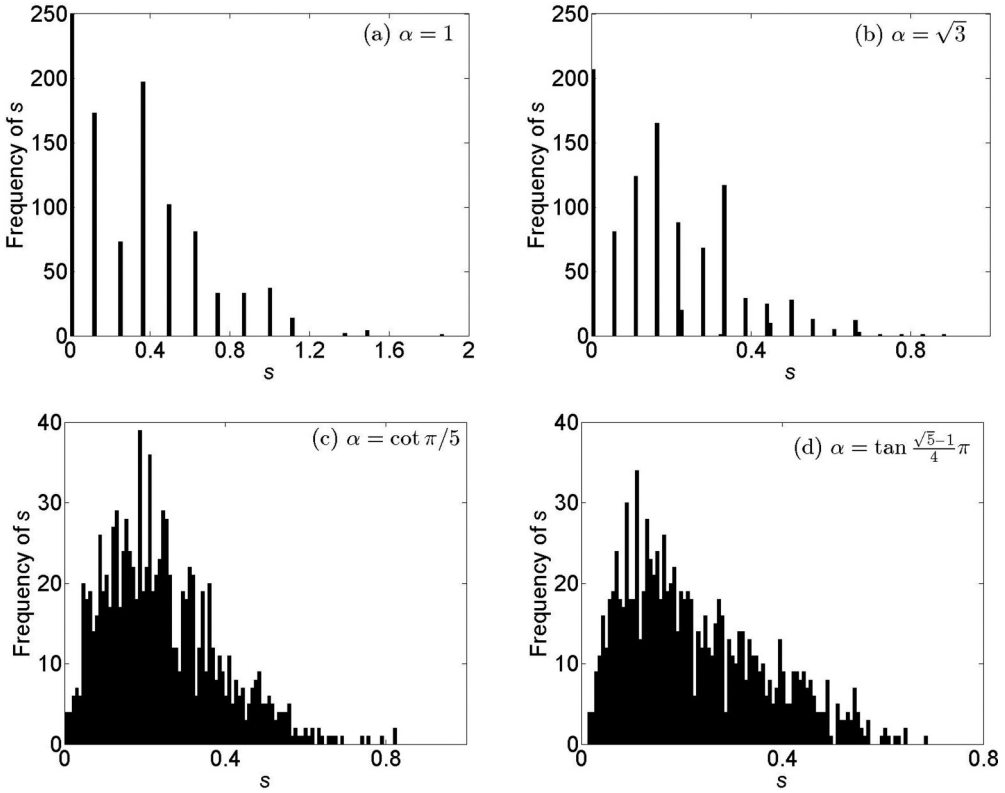

FIG. 2. Nearest spacing distribution of eigenenergies. (a) $\alpha = 1$ and (b) $\alpha = \sqrt{3}$ are two integrable cases. (c) $\alpha = \cot(\pi/5)$ is pseudointegrable. (d) $\alpha = \tan \frac{\sqrt{5}-1}{4}\pi$ is chaotic. Calculations are done for the first 1000 energy levels.

Wigner-like: an almost-zero probability density at $s = 0$ and a peak density at $s = s_m \neq 0$. This feature indicates that condition (1) is always satisfied by a quantum chaotic system. There is no clear conclusion for condition (2), as the peak at nonzero s in the Wigner distribution seems to suggest that Eq. (2) is not satisfied by a quantum chaotic system. However, our following numerical results show that condition (2) is also largely satisfied by a quantum chaotic system.

The Hamiltonian matrix of the triangle billiard is diagonalized numerically for a set of α. Its NSDs for the first 1000 energy levels are shown in Fig. 2 for four typical values of α. As expected, two integrable cases, $\alpha = 1$ and $\alpha = \sqrt{3}$, have lots of degenerate energy levels, while the pseudointegrable and chaotic cases have few.

With the obtained eigenenergies we can compute ζ and ξ, the two parameters that we introduced to describe quantitatively how well the two conditions, Eq. (1) and Eq. (2), for ergodicity and mixing are satisfied in a given system. We first construct the two distribution functions $f(\epsilon)$ and $g(\Delta)$ and then compute ζ and ξ using Eq. (12) and Eq. (13). The distribution function $f(\epsilon)$ together with $g(\Delta)$ is constructed by binning the energy levels with a width $\delta\epsilon = \hbar/T$, where T is the total time of a dynamical evolution. For a dynamical evolution of time T, energy levels or spacings separated by $\delta\epsilon = \hbar/T$ can be regarded as the same. In our calculation, we use $T = 40$ in accordance with our numerical study of quantum dynamics in the next section.

The results are listed in Table I, where we see clearly that the values of ζ and ξ are strongly correlated with the classical integrability of the system. For integrable systems, both ζ and ξ are large. As α changes and the system becomes more chaotic, ζ decreases almost to 0, while ξ is reduced by about two orders of magnitude. These numerical results strongly suggest that the conditions, Eq. (1) and Eq. (2), are largely satisfied by chaotic systems.

The pseudointegrable systems are subtle. As one may already have noted in Fig. 2(c) and Table I, the pseudointegrable case $\alpha = \cot \pi/5$ behaves very much like a chaotic system. However, not all pseudointegrable systems has a chaotic NSD.

TABLE I. Degeneracy parameters ζ and ξ for different values of α. The first 1000 energy levels are used in the calculation. Integrable cases are followed by a superscript asterisk. Clearly, integrable cases have much larger ζ and ξ.

α	ζ	ξ
1*	0.588	300.89
1.007846	0.032	14.39
1.015675	0	8.86
1.077744	0	8.65
1.154062	0	9.25
1.376382	0	11.04
1.461725	0	11.72
1.662013	0.002	13.33
1.700000	0.004	13.89
1.718079	0.010	18.84
1.725067	0.084	40.85
1.732051*	0.414	167.03

Some pseudointegrable triangle billiards, such as the triangle with angles $(\pi/5,2\pi/5,2\pi/5)$, have Possion-like NSDs [37]. Because the peaks of their NSDs $p(s)$ are at $s=0$, which indicates large degeneracy, these triangle billiards should have large ζ and ξ, and they are not ergodic or mixing. This difference shows that the relation between quantum ergodicity and mixing and classical integrability is very subtle in the case of pseudointegrable systems.

V. QUANTUM DYNAMICAL BEHAVIOR

In this section we study the quantum dynamics of the triangle billiard for a set of typical values of α to see whether it exhibits ergodic or mixing behavior as described by Eq. (7) or Eq. (8), respectively, and how these dynamical behaviors are dictated by conditions (1) and (2) via parameters ζ and ξ.

To study the quantum dynamical behavior, we need to calculate the time evolution of a wave function. We use the method of eigenstate expansion. For an arbitrary initial wave function $\psi(x,y,0)$, we expand it in terms of the energy eigenstates of the Hamiltonian $\phi_k(x,y)$,

$$\psi(x,y,0)=\sum_k c_k\phi_k(x,y). \tag{16}$$

According to the Schrödinger equation, the time evolution of this initial wave function is given by

$$\psi(x,y,t)=\sum_k c_k e^{\frac{-iE_k t}{\hbar}}\phi_k(x,y). \tag{17}$$

As the expansion coefficients can be calculated easily as

$$c_k=\iint_{\Omega_1}\psi(x,y,0)\phi_k^*(x,y)dxdy, \tag{18}$$

once we have obtained the expansion coefficients c_k, we can generate the wave function at any time. In our study, we choose a Gaussian wave packet as an initial state,

$$\psi(x,y)=\frac{1}{\sqrt{4\pi\sigma^2}}e^{-\frac{1}{4\sigma^2}[(x-x_0)^2+(y-y_0)^2]}e^{-i2\pi(p_x x+p_y y)}, \tag{19}$$

where $x_0=0.5$, $y_0=0.3$, $p_x=5\cos(e\pi)$, $p_y=5\sin(e\pi)$, and $\sigma=0.02$. This initial state mainly occupies the first 1000 energy eigenstates.

It is sufficient to focus on the momentum of the system. For the initial condition in Eq. (19) we have exactly $\langle\vec{p}\rangle_E=0$. The quantum dynamical evolutions of $\vec{p}$ are shown in Fig. 3 for four typical values of α: $\alpha=1$, $\alpha=\sqrt{3}$, $\alpha=\cot\pi/5$, and $\alpha=\tan\frac{\sqrt{5}-1}{4}\pi$. It is clear that the evolution of $\vec{p}$ varies greatly with different values of α. Before we discuss it in detail, let us first recall the classical dynamics for these four cases. The cases with $\alpha=1$ and $\alpha=\sqrt{3}$ are integrable; $\alpha=\cot\pi/5$ is pseudointegrable and has only finite directions of $\vec{p}$ in classical dynamics, which means nonergodicity. The case with $\alpha=\tan\frac{\sqrt{5}-1}{4}\pi$ is nonintegrable but classically nonergodic [7].

Let us return to the quantum dynamics in Fig. 3. For the two integrable cases, the long-time average is apparently not equal to its microcanonical ensemble average, and the fluctuation is large as well. For other cases, the momentum quickly relaxes to its microcanonical ensemble average and has only small fluctuations. The relaxation time is very short and is about $\sim 10^{-1}$ in these cases. Up to $t=40$, we do not observe a revival or large deviation from the equilibrium value. These results demonstrate that the quantum dynamics for $\alpha=\cot\pi/5$ (the pseudointegrable regime) and $\alpha=\tan\frac{\sqrt{5}-1}{4}\pi$ are not only ergodic but also mixing. This is in stark contrast with their classical dynamics, which are not even ergodic. This suggests

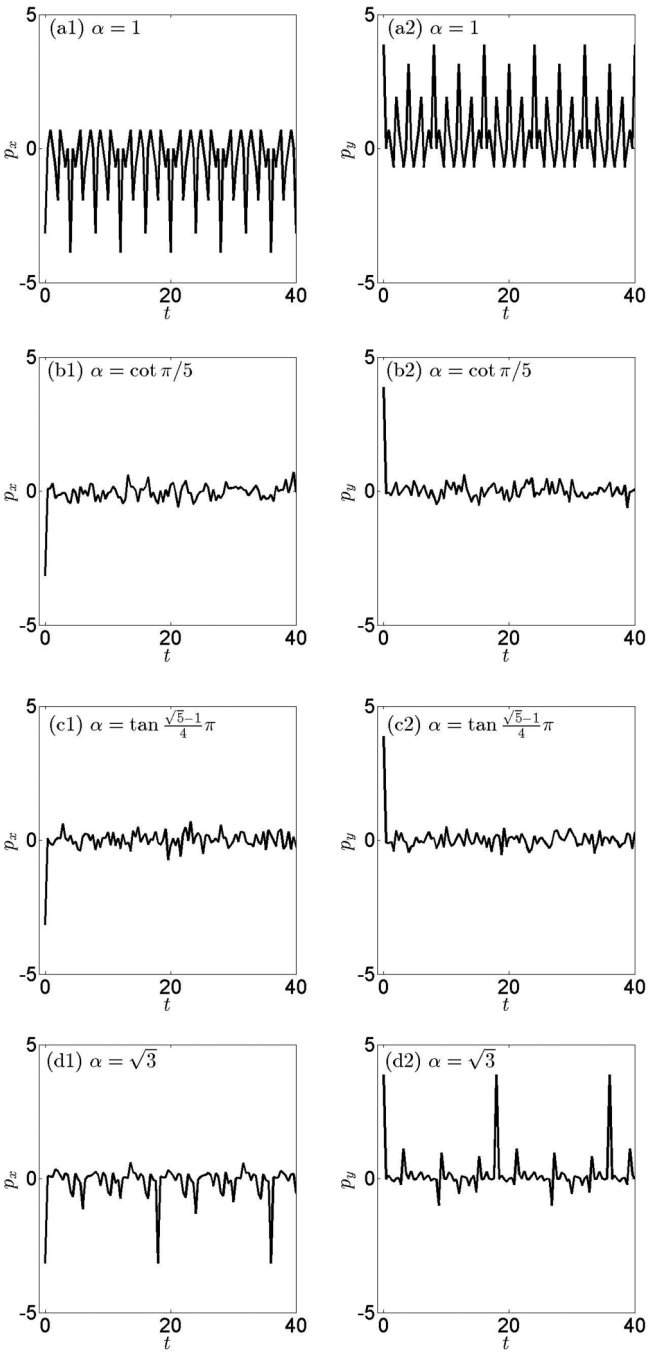

FIG. 3. Evolution of the momentum for different α values. $\alpha=1$ and $\alpha=\sqrt{3}$ are two integrable cases. $\alpha=\tan\frac{\sqrt{5}-1}{4}\pi$ is chaotic but nonergodic in classical mechanics [7]. $\alpha=\cot\pi/5$ is pseudointegrable.

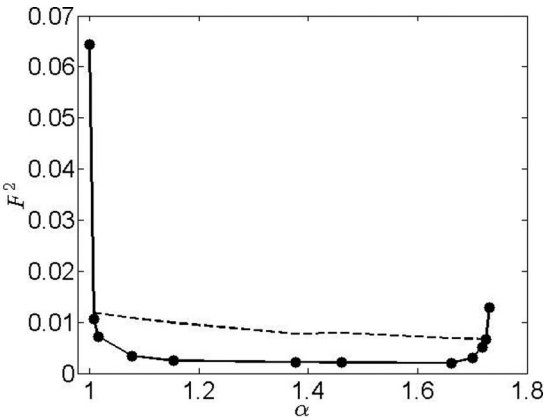

FIG. 4. Averaged relative fluctuations of the momentum via α. The vertical axis F^2 indicates the averaged relative fluctuation as defined in Eqs. (8) and (21). Filled circles are the numerical results; the solid line is a guide for the eyes; the dashed line is the upper bound $\mathrm{tr}\rho_{\mathrm{mc}}^2$ in Eq. (8).

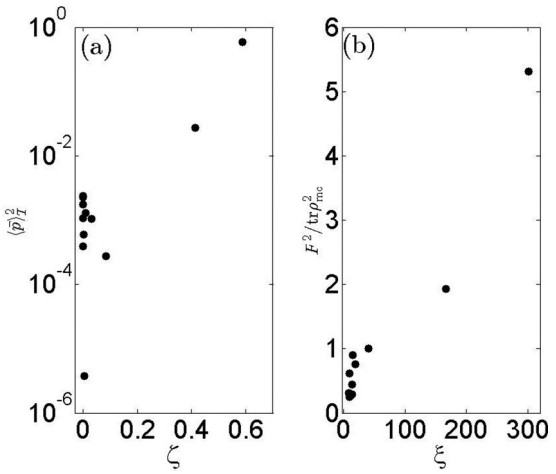

FIG. 5. (a) The square of time-averaged $\vec{p}$ at $T = 40$ with different ζ values. The vertical axis is on log scale. Note that $\langle\vec{p}\rangle_E = 0$. (b) Averaged relative fluctuation vs ξ. No mixing when $F^2/\mathrm{tr}\rho_{\mathrm{mc}}^2 > 1$.

that it is easier to have quantum ergodicity and mixing than in their classical counterparts.

In order to check quantitatively whether a quantum system is mixing, we need to calculate the time-averaged relative fluctuation. The averaged deviation of the momentum operator $\vec{p}$ in a given evolution time T is

$$\langle\sigma_{\vec{p}}^2\rangle_T = \frac{1}{T}\int_0^T \left|\langle\psi(t)|\vec{p}|\psi(t)\rangle - \sum_k |c_k^2|\langle\phi_k|\vec{p}|\phi_k\rangle\right|^2 dt. \tag{20}$$

Considering $E = \frac{\vec{p}^2}{2}$, the relative fluctuation of $\vec{p}$ is

$$F^2 = \frac{\langle\sigma_{\vec{p}}^2\rangle_T}{|\vec{p}|^2} = \frac{\langle\sigma_{\vec{p}}^2\rangle_T}{2E}. \tag{21}$$

The relaxation time scale is $\sim 10^{-1}$ and the oscillating period for integrable systems is $\sim 10^1$. Considering that a longer evolution time may lead to a large numerical error and unreliable result, we choose $T = 40$. This time length is much longer than the relaxation time, and it is also long enough for us to see if there are frequent recurrences.

The results of relative fluctuation for different values of α are shown in Fig. 4. The dashed line represents $\mathrm{tr}\rho_{\mathrm{mc}}^2$, the upper bound in Eq. (8). It can be clearly seen that for α away from 1 or $\sqrt{3}$, the averaged fluctuation is small, and the inequality, Eq. (8), is satisfied. This confirms the intuitive picture in Fig. 3 that the quantum dynamics is mixing. When α approaches the two integrable cases, $\alpha = 1$ and $\alpha = \sqrt{3}$, the averaged fluctuation becomes much larger, and the inequality, Eq. (8), is violated. In fact, in these two integrable cases, the averaged fluctuation reaches two local maxima. There is a rather rapid transition from mixing to nonmixing while the system is tuned from nonintegrable to integrable.

The quantum dynamic behavior shown in Fig. 3 is dictated by conditions(1) and (2). This is shown clearly in Fig. 5, where the square of the time-averaged momentum $\langle\vec{p}\rangle_T^2$ and its relative fluctuations are plotted against the two degeneracy parameters, ζ and ξ, respectively. It is clear from the figure that for systems with significantly nonzero ζ, the time average of the momentum significantly deviates from the microcanonical ensemble value. We can see a strong positive correlation between the relative fluctuation $F^2/\mathrm{tr}\rho_{\mathrm{mc}}^2$ and ξ as well. These results illustrate that systems with small ζ and ξ have ergodic and mixing quantum dynamics, respectively. Our definitions of quantum ergodicity and mixing with conditions (1) and (2) are legitimate.

VI. DISCUSSION AND CONCLUSION

Let us summarize what we have done. We have given our own definitions of ergodicity and mixing for quantum systems with conditions (1) and (2). It can be rigorously proved that these two conditions lead to quantum dynamical behaviors which are described by Eq. (7) and Eq. (8) and are reminiscent of classical ergodic and mixing dynamics, respectively. Through an example, the triangle billiard, we have further shown that although both conditions, Eq. (1) and Eq. (2), which are characterized by ζ and ξ, are related to classical integrability, there are differences. The most important is that a system whose classical dynamics is neither ergodic nor mixing can be both ergodic and mixing in its quantum dynamics.

Classical dynamics has an ergodic hierarchy [1,12,13], which is

$$\text{Bernoulli} \subset \text{Kolmogorov} \subset \text{Mixing} \subset \text{Ergodic}. \tag{22}$$

Now mixing and ergodicity have their quantum counterparts. In particular, we have a similar relation: quantum mixing systems are a subset of quantum ergodic systems. It is possible to expand this quantum ergodic hierarchy to three. We define

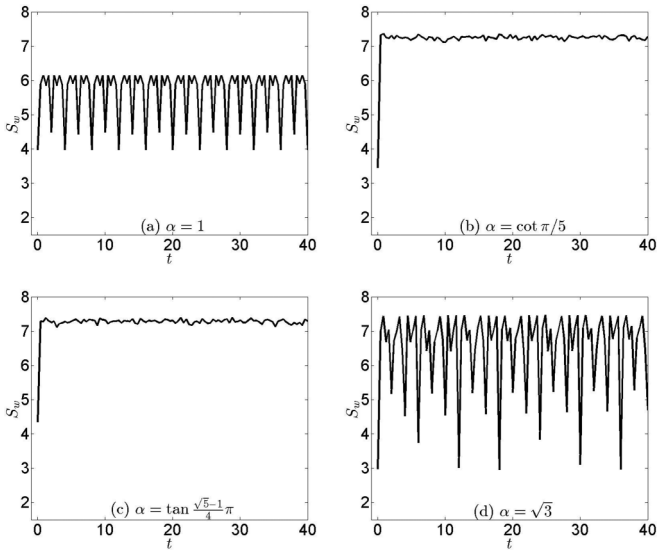

FIG. 6. Evolution of the entropy S_w for different values of α.

a quantum system as *H mixing* if the system satisfies

$$E_m + E_n - E_k - E_l = E_{m'} + E_{n'} - E_{k'} - E_{l'} \quad \text{and}$$
$$\{m,n\} \cap \{k,l\} = \emptyset \Rightarrow \{m,n\} = \{m',n'\}\{k,l\} = \{k',l'\}. \tag{23}$$

The "H" indicates the relation with quantum H theorem, which we show below. This condition implies that there is no degeneracy in the gaps of energy gaps. One can find the full implication of this condition in Ref. [15]. Here we briefly summarize. The entropy for a quantum pure state $\hat{\rho} \equiv |\psi\rangle\langle\psi|$ is defined as [15]

$$S_w \equiv -\sum_{\boldsymbol{q}_i,\boldsymbol{p}_j} \langle\psi|\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}|\psi\rangle \ln\langle\psi|\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}|\psi\rangle$$
$$\equiv -\sum_{\boldsymbol{q}_i,\boldsymbol{p}_j} \mathrm{tr}\left(\hat{\rho}\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}\right) \ln \mathrm{tr}\left(\hat{\rho}\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j}\right), \tag{24}$$

where $\boldsymbol{W}_{\boldsymbol{q}_i,\boldsymbol{p}_j} \equiv |w_{\boldsymbol{q}_i,\boldsymbol{p}_j}\rangle\langle w_{\boldsymbol{q}_i,\boldsymbol{p}_j}|$ is the projection onto Planck cells in quantum phase space at position $\boldsymbol{q}_i$ and momentum $\boldsymbol{p}_j$, and $\{|w_{\boldsymbol{q}_i,\boldsymbol{p}_j}\rangle\}$ is a complete set of Wannier functions. This entropy S_w will change with time. An inequality regarding the relative fluctuation of entropy S_w, similar to Eq. (8), was proved in Ref. [15] with condition (23). This inequality means that a quantum system with a low entropy S_w will relax dynamically to a state whose entropy S_w is maximized and stay at this maximized value with small fluctuations. This is illustrated by the triangle billiard in Fig. 6. In this figure we see that the entropy S_w of the integrable cases, for which condition (23) is not satisfied, fluctuates periodically with high amplitude and does not stay at the maximum value. For cases with $\alpha = \tan\frac{\sqrt{5}-1}{4}\pi$ and $\alpha = \cot \pi/5$, where Eq. (23) is largely satisfied, the entropy quickly relaxes to the maximum value and stays there with small fluctuations. These results demonstrate that a quantum system that satisfies condition is capable of equilibrating to a state where not only do its observables fluctuate around its equilibrium value at low amplitude, but also its entropy is maximized. This is what quantum H theorem states and, thus, the reason that we call such a quantum system H mixing. In this way we have a quantum ergodic hierarchy:

$$H \text{ mixing} \subset \text{Mixing} \subset \text{Ergodic}. \tag{25}$$

We do not call it quantum Kolmogorov, as we do not see an apparent connection to the classical Kolmogorov mixing system at this moment. It would be very interesting to find a quantum system which is H mixing but not mixing.

Finally, we conclude with expectations of future work to follow. We have given precise definitions of quantum ergodicity and mixing which are in accordance with our usual understanding of ergodicity and mixing. We have illustrated with single-particle billiard systems. It would be very interesting to further examine them in true many-body quantum systems [32,38], where the thermodynamics limit can be considered.

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APPENDIX A: CALCULATION OF EIGENENERGIES AND EIGENSTATES IN TRIANGLE BILLIARDS

We use the exact diagonalization method to calculate the eigenenergies and eigenstates: (i) choose an appropriate basis set; (ii) calculate the Hamiltonian matrix elements in the basis; and (iii) carry out numerical diagonalization, which results in the eigenenergies and eigenstates.

In order to reduce the numerical error to an acceptable range, we choose the basis as follows:

$$|m,n\rangle = \frac{2}{l\sqrt{\alpha}}\left(\sin\frac{m\pi x}{l}\sin\frac{n\pi y}{\alpha l} - \sin\frac{n\pi x}{l}\sin\frac{m\pi y}{\alpha l}\right). \tag{A1}$$

This choice is similar to that in Ref. [37]. This basis is complete and orthogonal. It is easy to check that all these base functions $|m,n\rangle$ are 0 on the boundaries of the triangle. The elements of the Hamiltonian matrix can be computed analytically,

$$\langle m_1,n_1|\hat{H}|m_2,n_2\rangle = \frac{h^2}{2ml^2}\left\{\left(m_2^2 + \frac{n_2^2}{\alpha^2}\right)[I(m_1,n_1,m_2,n_2) - I(n_1,m_1,m_2,n_2)]\right.$$
$$\left. -\left(n_2^2 + \frac{m_2^2}{\alpha^2}\right)[I(m_1,n_1,n_2,m_2) - I(n_1,m_1,n_2,m_2)]\right\}, \tag{A2}$$

where

$$I(m,n,p,q) = \int_0^1 dx \int_0^x dy \sin(m\pi x)\sin(n\pi y)\sin(p\pi x)\sin(q\pi y)$$

$$= \begin{cases} \frac{1}{8} & \text{if} \quad m=p \quad \text{and} \quad n=q, \\ \frac{1}{8\pi^2}(1-(-1)^{m+n+p+q})\left[-\frac{\{p-m+n+q\}^{-1}+\{q+n-p+m\}^{-1}-\{p+m+n+q\}^{-1}-\{n+q-p-m\}^{-1}}{q+n}\right. & \\ \left. +\frac{2}{(m+p)^2}-\frac{2}{(m-p)^2}\right] & \text{if} \quad m\neq p \quad \text{and} \quad n=q, \\ \frac{1}{8\pi^2}(1-(-1)^{m+n+p+q})\left[-\frac{\{p-m+n+q\}^{-1}+\{q+n-p+m\}^{-1}-\{p+m+n+q\}^{-1}-\{n+q-p-m\}^{-1}}{q+n}\right. & \\ \left. +\frac{\{p-m+q-n\}^{-1}+\{q-n-p+m\}^{-1}-\{m+p+q-n\}^{-1}-\{q-m-n-p\}^{-1}}{q-n}\right] & \text{if} \quad m\neq p \quad \text{and} \quad n\neq q, \end{cases} \tag{A3}$$

with the curly braces, $\{\cdot\}^{-1}$, representing

$$\{z\}^{-1} = \begin{cases} 0 & \text{if} \quad z=0, \\ \frac{1}{z} & \text{if} \quad z\neq 0. \end{cases} \tag{A4}$$

This notation is used only in Eq. (A3) to simplify the expression.

After the above derivation, we take a cutoff in n_1, n_2, m_1, m_2 and choose $h=m=l=1$ to calculate the elements of Hamiltonian matrix. The eigenenergies and eigenstates can be obtained after diagonalization of the Hamiltonian matrix. As the elements of the Hamiltonian matrix are explicit, the error of the eigenenergies and eigenstates mainly arises from the cutoff of n_1, n_2, m_1, m_2. In our calculation, the number of basis is set as 8500. Changing this number from 6000 to 10 000 causes only an $\sim$0.01% relative variation in eigenenergies (in units of h^2/ml^2). This indicates that the error in the numerical results of eigenenergies is around 0.01%, which is accurate enough for our analysis.

APPENDIX B: PROOFS OF LONG-TIME QUANTUM ERGODIC AND MIXING BEHAVIORS, EQ. (7) AND EQ. (8)

In this Appendix we provide the proofs of Eq. (7) and Eq. (8), which concern the long-time ergodic and mixing behavior in quantum systems, respectively. The original versions of the proofs can be found in Refs. [3,5,8,28].

Consider a quantum system that starts with the initial condition

$$|\psi(0)\rangle = \sum_n c_n |\phi_n\rangle , \tag{B1}$$

where the $|\phi_n\rangle$'s are the energy eigenstates. At time t, the wave function becomes

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar} |\phi_n\rangle . \tag{B2}$$

The corresponding density matrix is then

$$\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)| = \sum_{m,n} \rho_{nm} e^{-i(E_n-E_m)t/\hbar} |\phi_n\rangle\langle\phi_m| , \tag{B3}$$

where $\rho_{nm} = c_m^* c_n$. In an ergodic system where condition (1) is satisfied, we have

$$\begin{aligned} \langle\hat{\rho}(t)\rangle_T &= \left\langle \sum_{m,n} \rho_{nm} e^{-i(E_n-E_m)t/\hbar} |\phi_n\rangle\langle\phi_m| \right\rangle_T \\ &= \sum_{m,n} \rho_{nm} \langle e^{-i(E_n-E_m)t/\hbar}\rangle_T |\phi_n\rangle\langle\phi_m| \\ &= \sum_{m,n} \rho_{nm} \delta_{E_n,E_m} |\phi_n\rangle\langle\phi_m| \\ &= \sum_{m,n} \rho_{nm} \delta_{n,m} |\phi_n\rangle\langle\phi_m| \\ &= \sum_m \rho_{mm} |\phi_m\rangle\langle\phi_m| \\ &= \hat{\rho}_{\rm mc}, \end{aligned} \tag{B4}$$

which is exactly the microcanonical ensemble that we introduced in Eq. (5). Therefore, for an observable $\hat{A}$,

$$\langle\hat{A}\rangle_T = \langle \mathrm{tr}\hat{A}\hat{\rho}(t)\rangle_T = \mathrm{tr}[\hat{A}\langle\hat{\rho}(t)\rangle_T] = \mathrm{tr}\hat{A}\hat{\rho}_{\rm mc} = \langle\hat{A}\rangle_E . \tag{B5}$$

This is the proof of Eq. (7).

We now compute the standard deviation of $\hat{A}$:

$$\begin{aligned} \left\langle\sigma_A^2\right\rangle_T &= \langle |\langle\hat{A}(t)\rangle - \langle\hat{A}\rangle_E|^2\rangle_T \\ &= \langle |\langle\hat{A}(t)\rangle|^2\rangle_T - |\langle\hat{A}\rangle_E|^2 \\ &= \sum_{k\neq l, m\neq n} \rho_{lk}^* \rho_{nm} \langle e^{-i[(E_n-E_m)-(E_l-E_k)]/\hbar}\rangle_T A_{mn} A_{kl}^* . \end{aligned} \tag{B6}$$

When the quantum system is mixing, that is, both condition (1) and condition (2) are satisfied, we have

$$\begin{aligned} \left\langle\sigma_A^2\right\rangle_T &= \sum_{k\neq l, m\neq n} \rho_{kl}\rho_{nm}\delta_{E_n-E_m,E_l-E_k} A_{mn}A_{lk} \\ &= \sum_{k\neq l, m\neq n} \rho_{kl}\rho_{nm}\delta_{mk}\delta_{nl} A_{mn}A_{lk} \\ &= \sum_{m\neq n} \rho_{mn}\rho_{nm} A_{mn}A_{nm} \end{aligned}$$

$$= \sum_{m,n} |c_m|^2 |c_n|^2 A_{mn} A_{nm} - \sum_n |c_n|^4 |A_{nn}|^2$$
$$\leqslant \sum_{m,n} \rho_{mm} \rho_{nn} A_{mn} A_{nm}$$
$$= \mathrm{tr}\hat{A}\hat{\rho}_{\mathrm{mc}}\hat{A}^\dagger\hat{\rho}_{\mathrm{mc}} = \mathrm{tr}[(\hat{\rho}_{\mathrm{mc}}\hat{A}^\dagger)^\dagger(\hat{A}^\dagger\hat{\rho}_{\mathrm{mc}})], \quad \text{(B7)}$$

where we have used $A_{mn} = \langle\phi_m|\hat{A}|\phi_n\rangle$. We define a scalar product for two operators, $\hat{P}$ and $\hat{Q}$, as $\mathrm{tr}(\hat{P}^\dagger\hat{Q})$. Using the Cauchy-Schwartz inequality for operators with such a scalar product, we have [28]

$$\langle\sigma_A^2\rangle_T \leqslant \sqrt{\mathrm{tr}[(\hat{\rho}_{\mathrm{mc}}\hat{A}^\dagger)^\dagger(\hat{\rho}_{\mathrm{mc}}\hat{A}^\dagger)]\mathrm{tr}[(\hat{A}^\dagger\hat{\rho}_{\mathrm{mc}})^\dagger(\hat{A}^\dagger\hat{\rho}_{\mathrm{mc}})]}$$
$$= \sqrt{\mathrm{tr}\left(\hat{A}^\dagger\hat{A}\hat{\rho}_{\mathrm{mc}}^2\right)\mathrm{tr}\left(\hat{A}\hat{A}^\dagger\hat{\rho}_{\mathrm{mc}}^2\right)}$$
$$\leqslant \|\hat{A}\|^2\mathrm{tr}\hat{\rho}_{\mathrm{mc}}^2, \quad \text{(B8)}$$

where $\|\hat{A}\|^2 = \sup\{\langle\psi|\hat{A}^\dagger\hat{A}|\psi\rangle : |\psi\rangle \in \mathscr{H}\}$ is the upper limit of the expectation value of $\hat{A}^2$ in the Hilbert space. Finally, we have for the fluctuation

$$F_A^2 \equiv \frac{\langle\sigma_A^2\rangle_T}{\|\hat{A}\|^2} = \frac{\langle|\langle\hat{A}(t)\rangle - \langle\hat{A}\rangle_E|^2\rangle_T}{\|\hat{A}\|^2} \leqslant \mathrm{tr}\hat{\rho}_{\mathrm{mc}}^2. \quad \text{(B9)}$$

This is the proof of Eq. (8).

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